# Analytical Solutions to the Hulthén and the Morse Potentials by using the Asymptotic Iteration Method

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## Abstract

We present the exact analytical solution of the radial Schrödinger equation for the deformed Hulthén and the Morse potentials within the framework of the Asymptotic Iteration Method. The bound state energy eigenvalues and corresponding wave functions are obtained explicitly. Our results are in excellent agreement with the findings of the other methods.

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#### I. INTRODUCTION

In recent years, the energy eigenvalues and corresponding eigenfunctions between interaction systems have raised a great deal of interest in relativistic quantum mechanics as well as in non-relativistic quantum mechanics. The exact solution of the wave equations (relativistic or non-relativistic) is very important since the wave function contains all the necessary information regarding the quantum system under consideration. Analytical methods such as the super-symmetry (SUSY) [1] and the Nikiforov-Uvarov method (NU) [2] have been used to solve wave equations exactly or quasi-exactly for a given potential and these potentials are in general either the polynomial type like the Coulomb, the harmonic oscillator [3] or the exponential type such as the Eckart or Hulthén [3, 4, 6], Morse [5] or a combination of these potentials.

The Hulthén and Morse potentials we consider in this paper have a wide range applications. The Hulthén potential has a very important role in describing the bound states or continuum states between interaction particles in the relativistic quantum mechanics as well as the non-relativistic quantum mechanics. The Hulthén potential has been solved for the bound states with the NU [6], the SUSY [7, 8, 9, 10] and the shifted 1/N expansion [11] methods. It is also solved for the relativistic wave equations such as Dirac [12, 13, 14], Klein-Gordon (KG) [15, 16] and the Duffin-Kemmer Petiau (DKP) [17] equations.

The Morse potential has raised a great deal of interest over the years and has been one of the most useful models to describe the interaction between two atoms in a diatomic molecule. In this respect, Morse potential has been solved by the super-symmetry (SUSY) [1], the Nikiforov-Uvarov method (NU)[2], the hypervirial perturbation method (HV)[18], the shifted and modified shifted 1/N expansion methods [19] as well as the variational method [20].

Since these potentials have been extensively used to describe the bound and the continuum states of the interactions systems, it would be interesting and important to solve the non-relativistic radial Schrödinger equation for the Hulthén and Morse potentials. Recently, an alternative method called as the Asymptotic Iteration Method (AIM) for solving second-order homogeneous linear differential equation has been developed by Çiftçi et al. [21, 22] and has been applied to solve the non-relativistic radial Schrödinger equation or the relativistic Dirac equation.

In this paper, our aim is to solve the deformed Hulthén potential and the Morse potentials to obtain the energy eigenvalues and corresponding eigenfunctions within framework of the AIM. In the next section, the asymptotic iteration method (AIM) is introduced. Then, in section III, the Schrödinger equation is solved by the asymptotic iteration method for the deformed Hulthén potential and the Morse potential. The AIM results are compared with the findings of the other methods. Finally, section IV is devoted to the summary and conclusion.

### II. OVERVIEW THE ASYMPTOTIC ITERATION METHOD (AIM)

#### A. Energy Eigenvalues

AIM is briefly outlined here and the details can be found in references [21, 22, 23]. AIM is proposed to solve the second-order differential equations of the form

$$y'' = \lambda_0(x)y' + s_0(x)y \tag{1}$$

where  $\lambda_0(x) \neq 0$  and the prime denotes the derivative with respect to x. The variables,  $s_0(x)$  and  $\lambda_0(x)$ , are sufficiently differentiable. The differential equation (1) has a general solution [21]

$$y(x) = exp\left(-\int_{-\infty}^{x} \alpha(x_1)dx_1\right) \left[C_2 + C_1 \int_{-\infty}^{x} exp\left(\int_{-\infty}^{x_1} [\lambda_0(x_2) + 2\alpha(x_2)]dx_2\right) dx_1\right]$$
(2)

for sufficiently large k, k > 0, if

$$\frac{s_k(x)}{\lambda_k(x)} = \frac{s_{k-1}(x)}{\lambda_{k-1}(x)} = \alpha(x), \quad k = 1, 2, 3, \dots$$
 (3)

where

$$\lambda_k(x) = \lambda'_{k-1}(x) + s_{k-1}(x) + \lambda_0(x)\lambda_{k-1}(x)$$

$$s_k(x) = s'_{k-1}(x) + s_0(x)\lambda_{k-1}(x), \qquad k = 1, 2, 3, \dots$$
(4)

Note that one can also start the recurrence relations from k = 0 with the initial conditions  $\lambda_{-1} = 1$  and  $s_{-1} = 0$  [24]. For a given potential, the radial Schrödinger equation is converted to the form of equation (1). Then,  $s_0(x)$  and  $\lambda_0(x)$  are determined and  $s_k(x)$  and  $\lambda_k(x)$  parameters are calculated by the recurrence relations given by equation (4).

The termination condition of the method in equation (3) can be arranged as

$$\Delta_k(x) = \lambda_k(x) s_{k-1}(x) - \lambda_{k-1}(x) s_k(x) = 0 \qquad k = 1, 2, 3, \dots$$
 (5)

The energy eigenvalues are obtained from the roots of the equation (5) if the problem is exactly solvable. If not, for a specific n principal quantum number, we choose a suitable  $x_0$  point, determined generally as the maximum value of the asymptotic wave function or the minimum value of the potential [21, 24], and the approximate energy eigenvalues are obtained from the roots of this equation for sufficiently great values of k with iteration.

#### B. Energy Eigenfunctions

In this study, we seek the exact solution of radial Schrödinger equation for which the relevant second order homogenous linear differential equation takes the following general form [22],

$$y''(x) = 2\left(\frac{ax^{N+1}}{1 - bx^{N+2}} - \frac{(m+1)}{x}\right)y'(x) - \frac{wx^N}{1 - bx^{N+2}}y(x)$$
 (6)

the following general formula for the exact solutions for  $y_n(x)$  is given by [22],

$$y_n(x) = (-1)^n C_2(N+2)^n (\sigma)_{n} {}_2F_1(-n, \rho+n; \sigma; bx^{N+2})$$
(7)

where 
$$(\sigma)_n = \frac{\Gamma(\sigma+n)}{\Gamma(\sigma)}$$
,  $\sigma = \frac{2m+N+3}{N+2}$  and  $\rho = \frac{(2m+1)b+2a}{(N+2)b}$ 

# III. CALCULATION OF THE ENERGY EIGENVALUES AND EIGENFUNCTIONS

The motion of a particle with the mass m is described by the following Schrödinger equation:

$$\frac{-\hbar^2}{2m} \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] + V(r) \right) \Psi_{n\ell m}(r, \theta, \phi) = E \Psi_{n\ell m}(r, \theta, \phi)$$
(8)

The terms in the square brackets with the overall minus sign is the dimensionless angular momentum squared operator,  $\mathbf{L}^2$ . Defining  $\Psi_{n\ell m}(r,\theta,\phi) = u_{n\ell}(r)Y_{\ell m}(\theta,\phi)$ , we obtain the

radial part of the Schrödinger equation:

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)u_{n\ell}(r) - \frac{2m}{\hbar^2}\left[V(r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2}\right]u_{n\ell}(r) + \frac{2mE}{\hbar^2}u_{n\ell}(r) = 0$$
(9)

It is sometimes convenient to define  $u_{n\ell}(r)$  and the effective potential as follows

$$u_{n\ell}(r) = \frac{R_{n\ell}(r)}{r}, \quad V_{eff} = V(r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2}$$
 (10)

Since

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\frac{R_{n\ell}(r)}{r} = \frac{1}{r}\frac{d^2}{dr^2}R_{n\ell}(r)$$
(11)

The radial Schrödinger equation given by equation (9) follows that

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2m}{\hbar^2} \left[ E - V_{eff} \right] R_{n\ell}(r) = 0 \tag{12}$$

Instead of solving the partial differential equation (8) in three variables r,  $\theta$  and  $\phi$ , we now solve a differential equation involving only the variable r and the angular momentum parameter  $\ell = 0$  (s-state solution).

#### A. Deformed Hulthén Potential Case

The deformed Hulthén potential [4] is defined as

$$V_{DH}(r) = -Ze^2 \delta \frac{e^{-\delta r}}{1 - ae^{-\delta r}} \tag{13}$$

In this formula, Z,  $\delta$  and q are respectively the atomic number, the screening parameter and the deformation parameter determining the range for the deformed Hulthén potential. The deformed Hulthén potential reduces to the Hulthén potential form for q = 1, to the standard Wood-Saxon potential for q = -1 and to the exponential potential for q = 0.

Inserting the Hulthén potential given by equation (13) into equation 12 and using following ansatzs

$$-\varepsilon^2 = \frac{2mE}{\hbar^2 \delta^2}, \quad \beta^2 = \frac{2me^2 Z}{\hbar^2 \delta}, \tag{14}$$

and we apply a transformation to  $\delta r = x$  to the deformed Hulthén potential. The radial Schrödinger equation takes the following form:

$$\frac{d^2 R(x)}{dx^2} + \left(-\varepsilon^2 + \beta^2 \frac{e^{-x}}{(1 - qe^{-x})}\right) R(x) = 0$$
 (15)

If we rewrite equation 15 by using a new variable of the form  $y = e^{-x}$ , we obtain

$$\frac{d^{2}R(y)}{dy^{2}} + \frac{1}{y}\frac{dR(y)}{dy} + \left[-\frac{\varepsilon^{2}}{y^{2}} + \beta^{2}\frac{1}{y(1-qy)}\right]R(y) = 0$$
 (16)

In order to solve this equation with AIM, we should transform this equation to the form of equation 1. Therefore, the reasonable physical wave function we propose is as follows

$$R(y) = y^{\varepsilon}(1 - qy)f(y) \tag{17}$$

If we insert this wave function into the equation 16, we have the second-order homogeneous linear differential equations in the following form

$$\frac{d^2f(y)}{dy^2} = \left[\frac{(2\varepsilon q + 3q)y - (2\varepsilon + 1)}{y(1 - qy)}\right] \frac{df(y)}{dy} + \left[\frac{2\varepsilon q + q - \beta^2}{y(1 - qy)}\right] f(y) \tag{18}$$

which is now amenable to an AIM solution. By comparing this equation with equation 1, we can write the  $\lambda_0(y)$  and  $s_0(y)$  values and by means of equation 4, we may calculate  $\lambda_k(y)$  and  $s_k(y)$ . This gives:

$$\lambda_{0} = \left(\frac{2\varepsilon qy + 3qy - 2\varepsilon - 1}{y(1 - qy)}\right)$$

$$s_{0} = \left(\frac{2\varepsilon q + q - \beta^{2}}{y(1 - qy)}\right)$$

$$\lambda_{1} = \frac{2 + \beta^{2}qy^{2} - 8\varepsilon^{2}yq + 4\varepsilon^{2}y^{2}q^{2} - y\beta^{2} + 12q^{2}y^{2}\varepsilon + 11q^{2}y^{2} - 18\varepsilon yq + 6\varepsilon - 7qy + 4\varepsilon^{2}}{y^{2}(-1 + qy)^{2}}$$

$$s_{1} = \frac{(2\varepsilon q + q - \beta^{2})(-2 + 5qy - 2\varepsilon + 2\varepsilon yq)}{y^{2}(-1 + qy)^{2}}$$
(19)

 $\dots etc$ 

Combining these results with the quantization condition given by equation 5 yields

$$\frac{s_0}{\lambda_0} = \frac{s_1}{\lambda_1} \quad \Rightarrow \quad \varepsilon_0 = -\frac{1}{2} \frac{q - \beta^2}{q}$$

$$\frac{s_1}{\lambda_1} = \frac{s_2}{\lambda_2} \quad \Rightarrow \quad \varepsilon_1 = -\frac{1}{4} \frac{4q - \beta^2}{q}$$

$$\frac{s_2}{\lambda_2} = \frac{s_3}{\lambda_3} \quad \Rightarrow \quad \varepsilon_2 = -\frac{1}{6} \frac{9q - \beta^2}{q}$$

$$\dots etc$$
(20)

When the above expressions are generalized, the eigenvalues turn out as

$$\varepsilon_n = -\frac{1}{(2n+2)} \left( \frac{q(n+1)^2 - \beta^2}{q} \right), \qquad n = 0, 1, 2, 3, ...$$
(21)

Using equation 14, we obtain the energy eigenvalues  $E_n$ ,

$$E_n = -\frac{\hbar^2}{2m} \left[ \frac{\frac{me^2 Z}{\hbar^2}}{(n+1)q} - \frac{(n+1)\delta}{2} \right]^2, \qquad n = 0, 1, 2, 3, \dots$$
 (22)

In the atomic units ( $\hbar = m = e = 1$ ) and for Z = 1, equation 22 turns out to be

$$E_n = -\frac{1}{2} \left[ \frac{1}{\overline{n}q} - \frac{\overline{n}\delta}{2} \right]^2 \qquad \overline{n} = n+1 \qquad \overline{n} = 1, 2, 3, \dots$$
 (23)

It may thus be seen that the energy eigenvalue equation is easily obtained by using AIM. In order to test the accuracy of equation 23, we calculate the energy eigenvalues for Z=1, q=1 and several values of the screening parameter. The AIM results are compared with the Nikiforov-Uvarov [6] and the shifted 1/N [11] expansion methods in Table I. It may here be seen that the AIM results are in excellent agreement with the findings of the other methods.

Now, as indicated in Section II, we can determine the corresponding wave functions by using equation 7. When we compare equation 6 and equation 18, we find N=-1, b=q, a=q, and  $m=\frac{2\varepsilon-1}{2}$ . Therefore, we obtain  $\rho=2\varepsilon+2$  and  $\sigma=2\varepsilon+1$ . Having determined these parameters, we can easily find the eigenfunctions  $f_n(y)$  by using equation 7 as follows

$$f_n(y) = (-1)^n \frac{\Gamma(2\varepsilon_n + n + 1)}{\Gamma(2\varepsilon_n + 1)} {}_2F_1(-n, 2\varepsilon_n + n + 2; 2\varepsilon_n + 1; qy)$$
(24)

Finally, we can write the total radial wave function as below,

$$R_n = NC_n y^{\varepsilon_n} (1 - qy)_2 F_1(-n, 2\varepsilon_n + n + 2; 2\varepsilon_n + 1; qy)$$
(25)

where  $C_n = (-1)^n \frac{\Gamma(2\varepsilon_n + n + 1)}{\Gamma(2\varepsilon_n + 1)}$ .

#### B. Morse Potential Case

The Morse potential is defined as

$$V_{Morse}(r) = D_e \left( e^{-2\alpha x} - 2e^{-\alpha x} \right) \tag{26}$$

with  $x = (r - r_e)/r_e$  and  $\alpha = ar_e$ . Here,  $D_e$  and  $\alpha$  denote the dissociation energy and Morse parameter, respectively.  $r_e$  is the equilibrium distance (bound length) between nuclei and a

is a parameter to control the width of the potential well. Inserting equation 26 into equation 12 and using the following ansatzs

$$-\varepsilon^2 = \frac{2\mu r_e^2 E}{\hbar^2}, \qquad \beta^2 = \frac{2\mu r_e^2 D_e}{\hbar^2}$$
 (27)

The radial Schrödinger equation takes the following form:

$$\frac{d^2 R_n(x)}{dx^2} + \left(-\varepsilon^2 + 2\beta^2 e^{-\alpha x} - \beta^2 e^{-2\alpha x}\right) R_n(x) = 0$$
(28)

If we rewrite equation 28 by using a new variable of the form  $y = e^{-\alpha x}$ , we obtain

$$\frac{d^{2}R_{n}(y)}{dy^{2}} + \frac{1}{y}\frac{dR_{n}(y)}{dy} + \left[ -\frac{\varepsilon^{2}}{\alpha^{2}}\frac{1}{y^{2}} + \frac{2\beta^{2}}{\alpha^{2}}\frac{1}{y} - \frac{\beta^{2}}{\alpha^{2}} \right] R_{n}(y) = 0$$
 (29)

In order to solve this equation with AIM for  $\ell = 0$ , we should transform this equation to the form of equation 1. Therefore, the reasonable physical wave function we propose is as follows

$$R_n(y) = y^{\frac{\varepsilon}{\alpha}} e^{-\frac{\beta}{\alpha}y} f_n(y) \tag{30}$$

If we insert this wave function into the equation 29, we have the second-order homogeneous linear differential equations in the following form

$$\frac{d^2 f_n(y)}{dy^2} = \left(\frac{2\beta y - 2\varepsilon - \alpha}{\alpha y}\right) \frac{df_n(y)}{dy} + \left(\frac{2\varepsilon\beta + \alpha\beta - 2\beta^2}{y\alpha^2}\right) f_n(y) \tag{31}$$

which is now amenable to an AIM solution. By comparing this equation with equation 1, we can write the  $\lambda_0(y)$  and  $s_0(y)$  values and by means of equation 4, we may calculate  $\lambda_k(y)$  and  $s_k(y)$ . This gives (the subscripts are omitted):

$$\lambda_{0} = \left(\frac{2\beta y - 2\varepsilon - \alpha}{\alpha y}\right)$$

$$s_{0} = \left(\frac{2\varepsilon\beta + \alpha\beta - 2\beta^{2}}{y\alpha^{2}}\right)$$

$$\lambda_{1} = \frac{-3\beta\alpha y + 6\varepsilon\alpha + 2\alpha^{2} - 6\beta y\varepsilon - 2\beta^{2}y + 4\varepsilon^{2} + 4\beta^{2}y^{2}}{\alpha^{2}y^{2}}$$

$$s_{1} = 2\frac{\beta(2\varepsilon + \alpha - 2\beta)(-\alpha - \varepsilon + \beta y)}{\alpha^{3}y^{2}}$$
(32)

 $\dots etc$ 

Combining these results with the quantization condition given by equation 5 yields

$$\frac{s_0}{\lambda_0} = \frac{s_1}{\lambda_1} \quad \Rightarrow \quad \varepsilon_0 = -\frac{\alpha}{2} + \beta$$

$$\frac{s_1}{\lambda_1} = \frac{s_2}{\lambda_2} \quad \Rightarrow \quad \varepsilon_1 = -\frac{3\alpha}{2} + \beta$$

$$\frac{s_2}{\lambda_2} = \frac{s_3}{\lambda_3} \quad \Rightarrow \quad \varepsilon_2 = -\frac{5\alpha}{2} + \beta$$

$$\dots etc$$
(33)

When the above expressions are generalized, the eigenvalues turn out as

$$\varepsilon_n = \beta - (n + \frac{1}{2})\alpha$$
  $n = 0, 1, 2, 3, ...$  (34)

Using equation 27, we obtain the energy eigenvalues  $E_n$ ,

$$E_n = -\frac{\hbar^2}{2\mu r_e^2} \left[ \beta - (n + \frac{1}{2})\alpha \right]^2 \tag{35}$$

we calculate the energy eigenvalues of the  $H_2$  diatomic molecule. The AIM results are compared with those obtained by the hypervirial perturbation method (HV) [18], the shifted 1/N and modified shifted 1/N expansion methods [19] for the  $H_2$  diatomic molecule in Table II. As it can be seen from the results presented in these tables that the AIM results are in good agreement with the findings of the other methods.

Now, As indicated in Section II, we can determine corresponding wave function by using equation 7. When we compare equation 6 and equation 31, we find N=-1,  $a=\frac{\beta}{\alpha}$ , and  $m=\frac{2\varepsilon-\alpha}{2\alpha}$ . Therefore, we find  $\sigma=\frac{2\varepsilon}{\alpha}+1$ . For  $b\to 0$  we can take the limit in equation 7 using the limit relation

$$\lim_{b \to 0} {}_{2}F_{1}(-n, \frac{1}{b} + a; c; zb) = {}_{1}F_{1}(-n; c; z)$$
(36)

Consequently, the solution of equation 31 can easily find

$$f_n(y) = (-1)^n \frac{\Gamma(\frac{2\varepsilon_n}{\alpha} + n + 1)}{\Gamma(\frac{2\varepsilon_n}{\alpha} + 1)} {}_1F_1(-n, \frac{2\varepsilon_n}{\alpha} + 1; \frac{2\beta}{\alpha} y)$$
(37)

Thus, we can write the total radial wave function as below,

$$R_n(y) = N y^{\frac{\varepsilon_n}{\alpha}} e^{-\frac{\beta}{\alpha} y} {}_1 F_1(-n, \frac{2\varepsilon_n}{\alpha} + 1; \frac{2\beta}{\alpha} y)$$
(38)

where N is normalization constant.

#### IV. CONCLUSION

We have shown an alternative method to obtain the energy eigenvalues and corresponding eigenfunctions of the deformed Hulthén and the Morse potentials within the framework of the asymptotic iteration method. We have calculated the energy eigenvalues for Hulthén potential with Z = 1, q = 1 and several values of the screening parameter. The AIM results are compared with the Nikiforov-Uvarov [6] and the shifted 1/N expansion [11] methods in Table I. Furthermore, We have calculated the energy eigenvalues for  $H_2$  diatomic molecule and compared the hypervirial perturbation method [18], the shifted 1/N and modified shifted 1/N expansion methods [19] in Table II. As it can be seen from the results presented in these tables, the AIM results are in good agreement with the findings of the other methods.

The advantage of the asymptotic iteration method is that it gives the eigenvalues directly by transforming the radial Schrödinger equation into a form of  $y'' = \lambda_0(r)y' + s_0(r)y$ . The method presented in this study is a systematic one and it is very efficient and practical. It is worth extending this method to the solution of other interaction problems.

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${n}$	$-E_n(1/N)$ [11]	$-E_n(NU)[6]$	$-E_n(AIM)$		
	10( )	$\delta = 0.002$	<i>TU</i> ( )		
1	0.4990005	0.4990005	0.4990005		
2	0.1240020	0.1240020	0.1240020		
3	0.0545601	0.0545601	0.0545601		
4	0.0302580	0.0302580	0.0302580		
5		0.0012500	0.0012500		
$\delta = 0.01$					
1	0.4950125	0.4950125	0.4950125		
2	0.1200500	0.1200500	0.1200500		
3	0.0506681	0.0506681	0.0506681		
4	0.0264501	0.0264500	0.0264500		
5	0.0153128	0.0153125	0.0153125		
$\delta = 0.05$					
1	0.4753125	0.4753125	0.4753125		
2	0.1012503	0.1012500	0.1012500		
3	0.0333746	0.0333681	0.0333681		
4	0.0113035	0.0112500	0.0112500		
5		0.0028125	0.0028125		
	$\delta = 0.2$				
1	0.4049962	0.4050000	0.4050000		
2	0.0450856	0.0450000	0.0450000		
3		0.0005556	0.0005556		
4		0.0112500	0.0112500		
5		0.0450000	0.0450000		

TABLE I: The comparison of the AIM results (present work) with the findings of the 1/N [11] and NU [6] methods for the s-states energy eigenvalues of the Hulthén potential for several values of screening parameter  $\delta$ .

$n$ $\ell$	AIM	HV [18]	Modified Shifted 1/N	[19] Shifted 1/N [19]
0 0 -	4.47601	-4.47601	-4.4760	-4.4749
5 0 -	2.22052	-2.22051	-2.2205	-2.2038
7 0 -	1.53744	-1.53743	-1.5374	-1.5168

TABLE II: For the  $H_2$  diatomic molecule, the comparison of the energy eigenvalues (in eV) obtained by using AIM with other methods for different values of n. Potential parameters are  $D=4.7446eV,\,a=1.9425(A^0)^{-1},\,r_e=0.7416A^0,\,\hbar c=1973.29eVA^0$  and  $\mu=0.50391$ amu.